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Protocol for Reconciling Differences among Receptor and Dispersion Models

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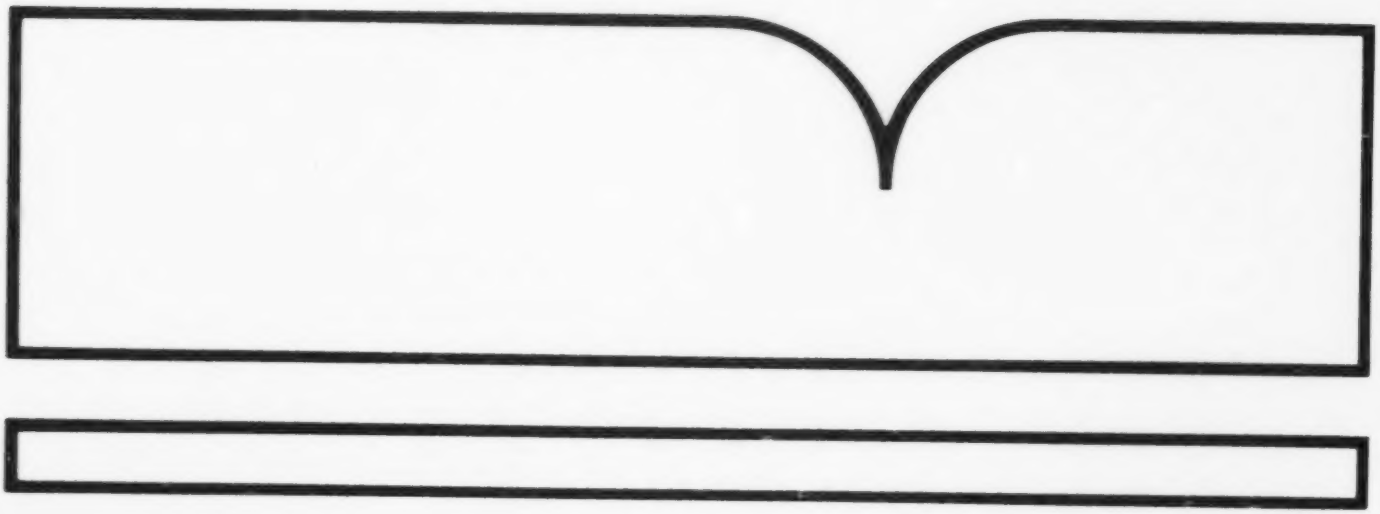

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16. ABSTRACT

The PM_{10} SIP Development Guideline, EPA-450/2-86-001, prepared by U. S. EPA, recommends that both dispersion models (DM) and receptor models, primarily the Chemical Mass Balance (CMB) model, be used to determine the contributing sources. When two or more independent methods, such as DM and CMB, are used to develop estimates for the contributing sources, differences are bound to occur.

This protocol consists of an eight step procedure for examining and reconciling differences in model estimates an a systematic, justifiable way. The steps outline a procedure for intercomparison of results, model refinement, recomparison and development of final model estimates.

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PROTOCOL FOR RECONCILING DIFFERENCES AMONG RECEPTOR AND DISPERSION MODELS

By

Air Management Technology Branch
Monitoring And Data Analysis Division

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Radiation
Office of Air Quality Planning and Standards
Research Triangle Park NC 27711

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INTRODUCTION

The PM_{10} SIP Development Guideline recommends that both Chemical Mass Balance (CMB) and Dispersion Models (DM) be used to determine the relative importance of various sources in contributing to ambient PM_{10} concentrations, provided the models are applicable.[1] Dispersion model applicability is discussed in Section 11.2.2 of the Guideline on Air Quality Models and in the Interim Procedures for Evaluating Air Quality Models.[2,3] The CMB applicability is discussed in the Protocol for Applying and Validating the CMB Model.[4]

Additionally, the PM_{10} SIP Development Guideline provides for the use of other receptor analyses to corroborate CMB and DM estimates. These other methods include optical or automated scanning electron microscopy (OM, ASEM), microinventory, factor analysis (FA), multiple linear regression (MLR), and trajectory analysis (TA), as discussed an Appendix A to the SIP Development Guideline. Use of several methods is desirable, because it yields estimates of source contributions from several perspectives, based on different assumptions and data. This approach greatly enhances the likelihood that the nature of an ambient PM_{10} problem is correctly understood. However, systems which rely on different measurements or use of different estimation parameters will likely yield different results. The differences may be negligible, but occasionally the differences may be large enough to require that they be reconciled.

The protocol summarized in this report consists of an eight-step procedure for examining and reconciling differences in model estimates in a systematic, justifiable way. This procedure is illustrated in Appendix A. The emphasis is on CMB and DM reconciliation, primarily because the SIP Development

Guideline identifies CMB as the principal receptor modeling approach for use in preparing SIP's for PM_{10}. Nevertheless, this protocol is intended to be general enough so that the results of other methods (e.g., "OM," "ASEM," or "MLR") could be reconciled in the same manner. (In fact, OM is used in the example in Appendix A.)

There are at least three generic cases which require model differences to be resolved (reconciled). The first case is when the results strongly suggest that at least one of the models has a significant error. The second case is when the model estimates are not disparate, but the overall uncertainty is judged to be large. Resources devoted to further refinement of the models and data bases might significantly reduce the uncertainties. The third case, a very common one, includes situations where one model is better for some source types, and another is better for other source types. Refinement of the final source contribution estimates should be cognizant of the suitability of each model to the suspect sources. Trijonis reports that the literature assumes that CMB models are more reliable than dispersion models for quantifying the impact of source categories (i.e., steel mills, power plants, woodstoves, road dust).[5] According to Trijonis, this may be because the CMB is tied directly to the ambient data that are being apportioned. The CMB is limited to apportionment of source categories unless there is only one source of that category upwind on the sampling day. In contrast, the DM can deal explicitly with emissions from single, identifiable sources within the same source category. However, in order to do so, the DM must build on several potentially uncertain inputs (emissions data, meteorological data, and the transport-diffusion-transformation-deposition mechanisms). Thus, the CMB and DM are complementary in their approach to source apportionment and using both can reduce the limitations of each alone.

CMB-DM RECONCILIATION

The CMB-DM reconciliation process is based on the premise that the receptor and dispersion models provide independent estimates of source contributions, rely on different data bases, have different underlying assumptions, and have different strengths and weaknesses. Generally, other receptor methods are used first, then the CMB is performed and, finally, the DM is run. Figure 1 depicts the flow of information if this order is maintained. At each step, the results of the other analyses are used to corroborate the ongoing analysis. The use of other receptor methods to corroborate the CMB is shown on Figure 1 for completeness but is discussed elsewhere.[4]

The reconciliation of CMB-DM results should follow an eight-step protocol involving comparison, reverification of input data, refining the inputs to both models, and rerunning the model(s) if necessary. The reconciliation protocol described in the remainder of this document assumes that both the dispersion model and CMB have been determined to be applicable and that preliminary results have been obtained for both models. The reconciliation process ends with control strategy development using the dispersion model unless the dispersion model is found to be inconsistent with the majority of the physical data. In such case, the CMB along with other receptor models would be used with a proportional model to develop a control strategy.[1]

Protocol Step 1: Compare CMB and DM Results

There are several issues that must be resolved in order to compare CMB and DM results: (1) consideration of suitable periods for sampling and analysis, with particular emphasis on source emission variability and

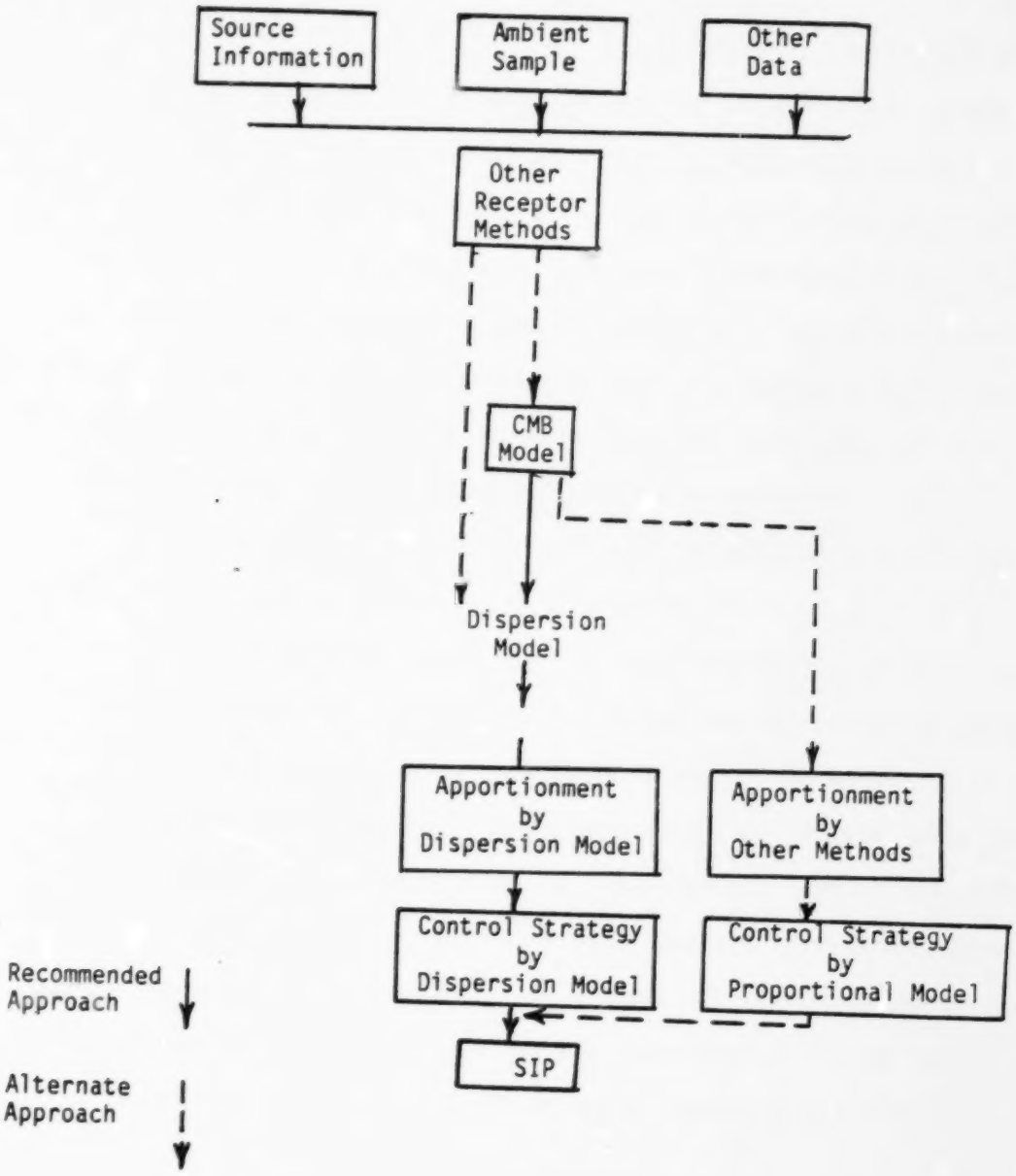

FIGURE 1. Information Flow For Source Apportionment And Control Strategy Development

meteorological conditions; (2) the issues of secondary particulate matter and background; and (3) grouping of the sources. These issues are discussed in the following paragraphs.

Selection of Sampling Periods for Analysis and Comparison. Attainment of the NAAQS is generally calculated based on ambient data. Ideally, for comparison purposes, the DM would be run for the actual monitoring period and CMB analyses would be available for each day during that same period. It is preferable that the CMB be performed on days selected randomly during the period. However, this ideal is virtually never achieved for numerous reasons of cost and practicality. For example, in assessing potential causes for not meeting the annual NAAQS, the DM may have to be run using meteorological data representing different years than those on which non-attainment is based. In that case, it would be necessary to perform CMB on a subset of days which are representative of the measured concentrations during the time period covered by the DM but also representative of the overall meteorology during that time period. In addition, the number of samples to be compared must reflect the seasonal differences in measured concentrations. In CMB applications relating to the annual NAAQS, a minimum of five samples in each quarter are considered necessary to obtain representative results.

For violations of the 24-hour NAAQS, it is preferable to apply the CMB model on the days on which "exceedances" of the NAAQS were observed. In this case, one would analyze and compare all observations greater than the level of the NAAQS. In order to obtain representative results, a minimum of five samples (e.g., the five highest values) should be compared. If there are fewer than five observed "exceedances" of the NAAQS, the five highest

values overall should be used so that the analysis is based upon a representative number of days. If a receptor model study were undertaken for a short time period, it must be shown that the period covered was generally representative of the types of source activity and meteorology which are associated with exceedances measured outside of the receptor model study. The source operating levels must be similar and the dispersion conditions and wind deviation during the shorter period must be such that the same sources would be expected to contribute to measured concentrations. The receptor data are particularly useful if exceedances are measured during the receptor study.

Unfortunately, a 24-hour emissions inventory appropriate for specific days may not be available or obtainable. Inventories usually contain annual average emissions. Thus, associating "dates" with the dispersion model results, which are based on annual emissions, could be risky. In this case, an "aggregate" comparison of the analysis results is recommended. To make an "aggregate" comparison, select a subset of dispersion model 24-hour estimates that has dispersion meteorology similar to that which occurred on the CMB analysis days (e.g., days with similar wind velocities and precipitation/cloud cover). Then, compare the source contributions for each CMB analysis with the average source contributions for the corresponding subset of dispersion modeled days.

Background and Secondary Particulate Matter. In many cases, the receptor model is used for source apportionment at urban or source oriented sampling sites, and the apportionment will include not only the "urban" contribution but also the background component which has been transported to the urban

area from elsewhere. In such cases, it is usually necessary to perform an analysis on a nearby background receptor so that the background or regional contributions to ambient PM observed at urban or source-oriented sites can be distinguished. This receptor analysis at a background site is necessary, for example, to distinguish between locally generated soil dust and that transported into the area. Receptor analyses from the background and other ambient monitors are then compared. Source categories that were identified on both urban and background monitors should be noted and estimated contributions of these sources at the study (urban) monitor should be reduced by the amount of their impact at the background site. In this process, one must carefully select the background days for receptor analysis to make sure they are "upwind" and are not impacted by local sources, and adjustments must be made to the CMB results prior to CMB-DM comparisons. Also, this reduction in urban contributions must be made carefully when background sources are chemically similar to sources in the urban area (e.g., soil and resuspended street dust), especially if the background site has considerable localized sources.

Grouping of Sources. CMB is usually only useful for identifying source categories contributing to ambient PM_{10}. In contrast, DM can identify contributions from individual sources. Thus, source contributions from the CMB and the DM must be grouped in such a way that contributions from similar sources can be assessed. The DM results are usually regrouped because the source chemical characteristics used in the CMB cannot usually be so done. Therefore, for the purpose of comparing DM results with CMB results, sources considered by the DM must be grouped into larger "categories" or source groups.

For example, perhaps a monitored sample was obtained from a coking operation. From a literature review or from experience, it is determined that the following operations at a steel making facility have emissions chemically similar to the coke sample:

Quenching

Pushing

Charging

Finished Coke Storage Pile

The "coke" source contribution calculated by the CMB would conceivably represent all of these specific sources. The DM output should group all of these sources together into a "coking" group; alternatively, the DM estimates for these sources could be manually grouped in a separate tabulation after the model is run.

Although groups are often arbitrarily selected, for purposes of CMB-DM model reconciliation, a little judicious planning can make the comparison of CMB with DM results fairly straightforward. This can enhance confidence in the models themselves if good agreement is found.

Grouping of DM sources is performed as follows:

(a) Review the detectable CMB source contribution categories to determine what they really include or represent. This should be documented with the best available references. For example, a "sea salt" source might include salt from ocean spray and also salt which was spread for snow control.[6]

(b) Review the Emission Inventory (EI) and decide which DM sources collectively comprise each CMB source category. Also, identify any unmodeled sources (e.g., continental dust, sea salt, etc.) that might be represented by the CMB source category.

(c) Combine the DM sources into groups that are consistent with CMB source categories.

(d) Identify any sources which were significant contributors in the CMB analysis but which were not in the DM emission inventory.

(e) Add these sources to the EI as appropriate.

(f) Rerun the DM.

(g) Make sure that the CMB has considered all nontrivial sources which were identified in the DM inventory. Rerun the CMB if necessary.

Comparison of Results. The grouping of sources described above allows a comparison of the DM and CMB estimates of the percentage contributions to the total calculated PM_{10} mass. First, establish an interval of + or - 30 percent around the DM results and + or - one standard error around the CMB results. If these intervals overlap, no further refinement is generally warranted. However, if the DM results imply a source group is a major contributor and the CMB results imply that it is not (or vice versa), the results must be reconciled, even if the comparison criterion (above) is met. If further refinement of the models or inputs are needed to meet the criterion, the procedure for doing so is described in the following section. Note that the + or - 30 percent interval about the DM is only for use in this intercomparison; it is not intended as a confidence interval for the DM.

Protocol Step 2: Verify Input Data in Both Models and Rerun if Necessary

This step ensures that the difference in CMB and DM results are not due to trivial or inadvertent problems with data entry. It should focus on the data entry process to verify that the models were run using the intended

data. The data review should include the ambient and source profile data, emissions data and meteorology. If all data are correct, skip to Step 4.

Protocol Step 3: Recompare Results

Any differences found in model estimates due to data entry should now be eliminated. Revised model results can now be compared, as discussed in Protocol Step 1. If the comparison criteria are not met, the next step is to reexamine model inputs, initially focusing on the CMB model.

Protocol Step 4: Refine CMB Model Inputs

This is an indepth review of the CMB model inputs, focused on those source groups where large differences between CMB and DM source category contribution estimates occurred. Because of the validation that the CMB application should have received, it is unlikely that there are any substantive CMB model input problems which were not apparent from the preliminary analyses.

However, insights available through the Dispersion Model analysis may highlight new problems or confirm suspicions that the modeler may have already had about weaknesses in the CMB that could not be previously substantiated. Also, it is appropriate to review the results of other receptor analyses at this point. This review may require modifying the model inputs or addressing collinearity.[4]

All measurements have some imprecision or uncertainty about them, and there will be some inherent underlying "noise" level in the data set which cannot be reduced by a reasonable allocation of time and resources. The user should review the CMB validation in light of the DM results.[4] If any weaknesses become apparent, address them to the extent time and resources permit, focusing on the source groups with disparate estimates. Then rerun

the CMB model, if any refinements were made. It is not sufficient to know just that a revision to a parameter will "fix" a discrepancy. Technical justification is required to document all changes that are made.

Protocol Step 5: Recompare Results

Any remaining differences found between CMB and DM model estimates are best addressed by closer examination of the dispersion model. If the comparison criteria in Step 1 are met, skip to Step 7.

Protocol Step 6: Refine Dispersion Model Inputs and Rerun

This is an indepth review of the dispersion model, focusing on those source groups (e.g., fugitive dust sources) for which large differences occur between DM and CMB. This review should include (1) the appropriateness of emissions data, which are based on the identification of sources and their locations, activity rates, emission factors and release heights; (2) meteorological data; and (3) underlying assumptions in the model itself and its dispersion, transformation, and removal algorithms. Reference 7 gives examples of factors that primarily affect individual source-to-monitor impacts:

- Erroneous emission data caused by such items as the omission of unknown sources from the modeling or the use of inaccurate throughput information.
- The use of inappropriate emission rates, such as the use of total particulate matter emission rates which include particle sizes larger than PM_{10} that settle out prior to impacting the monitoring site and are not collected by a PM_{10} sample if they do reach the receptor.
- Incorrect information concerning daily source operating parameters. For example, while a source may operate at 45 percent capacity on an annual basis, its actual mode of operation may be at 90 percent capacity for 50 percent of the days in a year.

- o Neglect or incorrect consideration of downwash from tall stack sources.
- o Neglect or incorrect consideration of particles resuspended by the wind or mechanical action.
- o Building interference causing source-to-receptor (i.e., source-to-monitor) geometry to be incompatible with Gaussian dispersion assumptions.
- o Local meteorology differing from that modeled. A typical problem is wind direction shift or channeling caused by buildings or topographic features.

In reference 7, Anderson suggests that these emissions and meteorological data problems can often be satisfactorily resolved by:

(a) identifying significant sources or source groups from the CMB results;

(b) assigning a "level of confidence" to emission and meteorological parameter estimates for each significant source or source group, based on engineering estimates. The confidence level information needed for this analysis may be found in Volume V of the Receptor Model Technical Series.[7] Ideally this analysis should be completed before the CMB and dispersion - models are run.

(c) revising the emission and meteorology parameter estimates, as appropriate. It is not sufficient to know just that a revision to a parameter will "fix" a discrepancy. Technical justification is required to document all changes that are made.

The pattern of discrepancies at different receptors may also aid in identifying potential inventory errors. For example, large under- or over-prediction by the dispersion model at a receptor very close to a source may suggest possible errors in source receptor geometry. Large overprediction at receptors far from a source would suggest an erroneous particle size

distribution in emission factors. Experience with dispersion models and emission inventories will play an important role in diagnosing potential inventory problems.

The dispersion model is then rerun, using the revised input parameters.

Protocol Step 7: Recompare Results and Evaluate the Dispersion Model

The revised dispersion model results are again compared with the CMB results to determine whether further modifications to the dispersion model or meteorological inputs are warranted.

Anderson provides examples of factors that are not typically addressed by the dispersion model that may cause systematic biases in model results. These factors are addressed in various nonguideline models that are currently available.

- Heat island effects which cause the actual near-source dispersion of elevated emissions to be greater than that modeled.
- Sea/land breeze and convergence zone effects.
- Effects caused by the fumigation of tall stack emissions.
- Effects caused by the development of thermal internal boundary layers (TIBL) over areas with varying surface heating characteristics.

Remedies to these problems might include acquisition of additional meteorological data, choice of different model options or modification of dispersion algorithms to meet local disperson conditions and source characteristics. Such problem specific model modifications may prove a time and cost effective alternative to additional sampling and analysis. These remedies should be applied to the extent permitted by time and resource constraints.

Protocol Step 8: Final Model Estimates as Basis for Control Strategy

The reconciliation process should help improve both the initial DM and CMB results so that the differences between models are resolved. If this is the case, it is recommended that the DM model be used for control strategy development. If, however, it is clearly evident that the dispersion model results are inconsistent with the majority of the physical data and cannot be made consistent through justifiable modifications to the input data, the CMB estimates should be used as the basis for control strategy development. It is better to use the results of the method believed to provide the best results, rather than average the results of two or more methods.

EXAMPLE

Appendix A describes the application of this protocol to an industrial area. The example includes the use of preliminary analyses including pollution rose and microinventory, dispersion modeling using the Industrial Source Complex-Short Term Model (ISCST), and receptor modeling using the Chemical Mass Balance (CMB) and optical microscopy (OM).

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APPENDIX A - EXAMPLE APPLICATION OF PROTOCOL IN AN INDUSTRIAL AREA

INTRODUCTION

This section describes an example application of the protocol for a nonattainment site located within an industrial area. The example was adapted from an actual environmental case study and modified where necessary to enable its use with this protocol.[8] All modifications were cognizant of what could and would have actually been done in the reconciliation had time and resources permitted.[9] In this example, the causes of the elevated concentrations of PM_{10} are not apparent due to the large number of point and area sources located relatively close to the monitoring site. Based strictly on the emission inventory, stack and fugitive dust emissions from a large steel mill as well as traffic generated resuspended road dust appear to be potentially large contributors to the particulate matter loadings observed at the monitoring site. An investigation, which includes ambient and source data collection, optical microscopy (OM), pollution rose (a form of trajectory analysis), dispersion modeling (DM) and chemical mass balance (CMB) modeling efforts, was conducted in order to apportion the source impacts with the level of confidence necessary for making control strategy decisions. The results are reconciled using the eight-step process previously described.

The industrial site PM_{10} source apportionment example presented in this section is compiled primarily from experience gained from assessing source impact at a single monitoring site. The purpose of this example is to illustrate use of the eight-step reconciliation protocol described in this document. Therefore, the identity of the site and details of the OM, CMB, and DM analyses are unimportant to the objective of the example and are not presented in detail.

OVERVIEW OF THE SOURCE APPORTIONMENT STUDY

A combined receptor and dispersion modeling study was implemented with the objective of identifying and quantifying impacts of the sources contributing to violations of the PM_{10} NAAQS recorded at a monitoring site. To supplement the emission inventory, pollution concentration roses were prepared using data for eight TSP monitoring sites located near the PM_{10} monitoring site. The pollution roses clearly indicate that the major sources of TSP are located in the quadrant south of the PM_{10} monitor. That is, a preponderance of the high 24-hour average TSP measurements correspond with days having resultant winds from the south. This preliminary receptor analysis suggests that additional emphasis should be placed on characterizing steel mill related contributions because the steel mill is the largest source of particulate emissions located nearby and south of the monitoring site.

Receptor Modeling Data Collection Tasks

The ambient data base consisted primarily of: (1) ambient PM_{10} samples collected for 1 year on an every-6th-day schedule; and (2) hourly measurements of wind direction, wind speed, and temperature at the PM_{10} monitoring station. The PM_{10} samples were collected on quartz fiber filters using a size-selective high volume (SSHV) sampler. In addition, for 1 month a dichotomous sampler was in operation at the monitoring site and collected several 24-hour coarse and fine fraction samples on Teflon filters. The results of the PM_{10} monitoring program provided an annual average PM_{10} concentration of 65 $\mu g/m^3$ as well as four exceedances of the 24-hour average PM_{10} standard of 150 $\mu g/m^3$.

A site visit was made to compile a microinventory of emission sources. The microinventory procedure consisted of determining the nature, location and spatial extent of all fugitive dust sources within one-quarter mile of the PM_{10} monitoring station. The information was then used to calculate the emission rates for input to a dispersion model. Source types included unpaved roads, paved streets, railroads, and two coal storage piles. Emission rates were determined using published emission factors together with the source area and traffic volumes.

As part of the site visit, samples of emitted materials were collected from six sources in the general vicinity of the site which had been identified as potentially important contributors to PM_{10}. The samples were subsequently analyzed to provide source profiles for use in the CMB model. The sources which were sampled included: a steel mill (blast furnace, coke oven, and basic oxygen furnace); two road shoulders (one near the monitoring site and one near an inoperative lead plant); and an agricultural processing plant (potash, corn gluten pellets, and soybeans).

Two subsets of the ambient PM_{10} filters were selected for analysis as discussed above. Subset A contained the filters from 20 sampling days which were selected to be representative of the annual average conditions at the monitoring station. The average PM_{10} concentration calculated from the filters in subset A was 67 $\mu g/m^3$, which compares well with the annual average calculated from all the filters (65 $\mu g/m^3$). Subset B contained the samples from the 4 days on which exceedances of the 24-hour average NAAQS were recorded plus the highest nonexceeding day (a total of 5 days). This subset was chosen to guide control strategy development related to the 24-hour standard.

Two multi-elemental characterization techniques were applied to the source and ambient filters. X-ray fluorescence (XRF) was performed on the Teflon filters, and Plasma Emission Spectroscopy (PES) was employed for the quartz filters. The following species were analyzed: Na, Mg, Al, Si, K, Ca, Ti, V, Mn, Fe, Zn, Br, Pb, EC and SO_4. The elemental carbon (EC) content of the samples was determined by the optical attenuation analysis method. In addition to the chemical characterization procedures, optical microscopy was applied to several of the ambient samples. Optical microscopy, which provides reliable particle identifications and semi-quantitative source contribution estimates, was used as a QA check on the receptor modeling source identifications and to aid in the receptor/dispersion model reconciliation process.

Receptor modeling was performed for this study using the Chemical Mass Balance (CMB) model.[4,10] The CMB model requires an input file containing the measured ambient concentrations of the elements for which the samples were analyzed. This requirement was fulfilled by transforming the results of the ambient filter analysis into the format specified by the CMB model. In addition, the CMB model requires a file containing the source compositions reported as the elemental mass fractions. A source composition file in CMB specified format was compiled. The file contained the elemental composition of the resuspended local sources as well as a number of source profiles which were extracted from EPA's Source Composition Library.[6] The emission inventory and the microinventory were used to select sources for consideration in the CMB.

Dispersion Modeling Data Preparation

The emission inventory of all the point sources in the two counties surrounding the PM_{10} monitoring site was obtained. A total of 140 point sources

were included in the inventory. The point source inventory was modified for use in modeling PM_{10} impacts by applying source specific PM_{10}/TSP emission ratios to the TSP emission factors which were originally contained in the inventory.

The Industrial Source Complex Short-Term (ISCST) model was used for this investigation. ISCST was used because it is applicable to the dispersion conditions found in the study area, and it contains several features that improve the source apportionment process. Two potentially advantageous features of ISCST are the ability to: (1) model microinventoried fugitive dust sources as volume sources; and (2) calculate the combined impact for selected groups of sources. This latter feature greatly decreases the manipulations necessary to transform dispersion and receptor modeling results into comparable formats providing basis for comparisons.

Two receptor oriented approaches are utilized in this example: the CMB model and the optical microscopy technique. CMB modeling analyses were performed on the data obtained from filters contained in subsets A and B described in Section 2.1. The modeling procedure consists of obtaining a solution using the CMB procedures found in reference 4.

Two SSHV samples, two coarse fraction dichotomous samples, and one fine fraction dichotomous sample (ambient samples) underwent optical microscopic analysis to confirm the CMB source identifications. In addition, the results of the particle counting performed as part of the microscopic analysis are used to calculate semi-quantitative source contribution estimates.

As part of the CMB modeling procedure, efforts are made to develop information which could be used to confirm or refute the validity of the CMB results. This information can be classified into four categories: (1) applicability of the model to the situation; (2) evidence of adherence or deviation from model assumptions by examination of the summary statistics resulting from the use of model assumptions; (3) stability of source impact estimates with respect to minor changes in the CMB model fitting parameters; and (4) comparisons with preliminary analyses (e.g., pollution rose, OM and microinventory analyses). By evaluating the CMB results on the basis of the above four categories, the CMB analyses are determined to be valid.

Background concentrations are defined as that portion of the measured ambient levels that is not attributable to emissions within the study area. To estimate the appropriate background concentrations for the dispersion model, an eclectic pollution rose* was developed using data from TSP monitoring stations located outside the study area. Data were used only from the days having persistent winds blowing into the study area from the direction of the background TSP stations. An average TSP concentration of 26 $\mu g/m^3$ was determined to be attributed to sources outside the study area. Application of the site-specific PM_{10}/TSP ratio (0.57) yields an average background PM_{10} concentration of 15 μgm^3. Background concentrations were also estimated for each wind sector using this method.

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*The term "eclectic pollution rose" is used to describe a rose developed by compositing the data from several monitors surrounding the urban area such tnat the eclectic rose reflects concentrations only when the wind is blowing into the urban area.

THE EIGHT-STEP RECONCILIATION PROCESS

Step 1 - Compare DM and CMB Results

The dispersion model simulation results for time periods corresponding to the PM_{10} sampling schedule at the monitoring station were compared with measured PM_{10} air quality data. This comparison suggests that the ISCST is underpredicting PM_{10} concentrations at the monitoring site. Comparison of the predicted PM_{10} with the measured PM_{10} minus estimated background PM_{10} concentrations provided an indication that the model was underpredicting.

The source contributions from the DM and CMB were grouped in such a way that they could be compared. This was actually done to some extent before the ISCST was run by examining the emission inventory. The emission inventory contained the name of each plant and a description of each emission source. This information was used to develop a preliminary tabulation of the types of materials (e.g., specific source chemistry) emitted by each source. The many types of emitted materials were then associated with 1 of 17 general categories which were determined to be consistent with the source profiles used in the CMB analysis. Each of the 140 point sources and 25 volume sources was assigned a code corresponding to 1 of the 17 categories. Some overlap and "juggling" of categories was inevitable but a reasonably good preliminary grouping was made. The results are presented in Table A.1. Adjustment to this preliminary grouping may be necessary in some cases.

The source contribution estimates provided by the CMB and ISCST models for subset A (annual average) and subset B (samples violating the 24-hour NAAQS) are compared in Table A-2. The basic oxygen furnace and steel blast furnace groups were combined for the same reason. The results of the two

TABLE A-1

TYPES OF EMISSIONS ASSIGNED TO EACH SOURCE
GROUP IN THE DISPERSION MODELING ANALYSES

Group Number	Type of Emission
1	Oil and Gas Combustion
2	Coal Combination
3	Wood-fired Boilers
4	Agricultural Products Handling
5	Coking Operations
6	Coal Handling
7	Steel Blast Furnace and BOF
8	Paint Production
9	Cement and Limestone
10	Motor Vehicle Exhaust and Lead Processes
11	Sand and Bentonite
12	Aluminum Production
13	Zinc Processing
14	Tire Production
15	Oil Refining
16	Fertilizer
17	Road Dust, Soil, and Motor Vehicle Exhaust

TABLE A-2
COMPARISON OF INITIAL RESULTS BY ISCST AND CMB FOR SUBSETS A AND B (ug/m^3)

Source Categories	(Representing Annual Average) Subset A ISCST	CMB	(Average of 5 Highest 24-hr Exceedances) Subset B ISCST	CMB
Oil & Gas Combustion	1.6	--	2.0	--
Wood-fired Boilers	0.2	3.2 (1.4)	0.8	5.6 (2.1)
Coal Combustion	0.6	2.8 (1.1)	1.2	8.0 (3.2)
Coking Operations	1.4	8.6 (4.2)	4.0	23.2 (8.7)
Blast Furnace[a]	0.6	12.0 (3.5)	2.0	33.6 (8.9)
Basic Oxygen Furnace[a]		3.8 (1.5)		10.4 (2.7)
Coal Handling	0.3	--	0.6	--
Agricultural Prod. Handling	1.1	--	1.6	--
Paint Production	--	--	0.8	--
Cement & Limestone	1.9	--	1.9	--
Sand & Bentonite	1.2	--	1.7	--
Aluminum Production	--	--	0.4	--
Zinc Processing	0.8	--	0.6	--
Oil Refining	0.6	--	1.6	--
Fertilizer	--	--	0.8	--
Tire Production	--	--	2.2	--
Motor Vehicle Exhaust	15.1	2.4 (0.8)	2.6	2.4 (0.9)
Road Dust & Soil		30.0 (7.2)	31.2	79.2 (20.3)
Secondary $(NH_4)_2SO_4$	--	15.0 (2.5)	--	27.4 (5.0)
Background	15.0	--	32.0	--
Total	45.4	77.8	89.0	189.8
Measured	67.0	67.0	162.0	162.0

[a] Estimated as a single source by the ISCST because of lack of detail in the emission inventory.

NOTE: Numbers in parentheses indicate one standard error in the CMB analysis.

models display reasonable agreement in two categories: (1) the background estimates used by ISCST are approximately equal to the secondary sulfate values estimated by CMB; and (2) resuspended road dust is listed as a major source of PM_{10} by both methods. In addition, the similarities and differences between CMB and ISCST are consistent between subsets A and B. Aside from the relatively few similarities which have been enumerated, many differences between the CMB and ISCST results are evident. For example, ISCST underpredicts the measured mass and CMB overpredicts the measured mass. Furthermore, ISCST assigns contributions to several source categories which were not identified by the CMB method. Finally, CMB and ISCST estimated substantially different impacts for wood-fired boilers, coal combustion, the road dust and motor vehicle exhaust combination and the steel mill related emissions from coking operations, blast furnace, and basic oxygen furnace. Unfortunately, Table A-2 does not reflect conclusions drawn from any OM analysis, because the OM analysis is available for only 2 days.

As a result of this comparison, four cases were identified (based on comparison model results as discussed in Step 1 of the Protocol) where additional model refinements may be necessary:

Case 1. The combined contributions of motor vehicle exhaust and resuspended road dust, as estimated by CMB and ISCST, were in major disagreement.

Case 2. A significant disagreement exists between the CMB and ISCST estimates of the coal combustion impacts.

Case 3. CMB estimates wood-fired boilers to be a much larger contributor to PM_{10} than does ISCST.

Case 4. There is a major disagreement between CMB and ISCST for steel mill related impacts (i.e., coking operations, blast furnace and basic oxygen furnace source categories).

Each case is discussed below under the appropriate step in the reconciliation process.

Steps 2 and 3 - Verify Input Data, Rerun Models and Recompare Results

A review of the input data for both models indicated that they were indeed using the data that were intended. None of the four cases were related to inadvertent errors in data input.

Step 4 - Refine CMB Model Specification

Operationally, all four cases identified in Step 1 are reviewed at this point. Only case 1 was found to be related to the CMB inputs. Thus, discussion of the other three cases is included under step 6. Tables A-3 and A-4 compare the source impacts estimated by ISCST, CMB and optical microscopy for the 2 days, October 1, 1983 and October 25, 1983, when OM analysis was performed.

Case 1. The combined contributions of motor vehicle exhaust and resuspended road dust, as estimated by CMB and ISCST, were in major disagreement.

The first step taken to reconcile the disagreement between CMB and ISCST with respect to the combined impact of vehicle exhaust and road dust was to re-examine the comparisons between OM, CMB, and ISCST. This is shown in Tables A-3 and A-4 for the 2 days for which OM data are available. In this case, OM was found to agree very well with ISCST. The CMB input data were then evaluated for potential errors related to estimating road dust and vehicle exhaust. The coarse fraction filter on which the resuspended road dust source sample was collected appeared to have lost a substantial fraction of the sample

TABLE A-3

COMPARISON OF THE RECEPTOR AND DISPERSION MODEL RESULTS FOR THE OCTOBER 1, 1983 PM_{10} SAMPLES

Dispersion Modeling Source Groups	Optical Microscopy Source Categories	CMB Modeling Source Types	Modeled Concentrations ($\mu g/m^3$)						
			Dispersion Modeled Impacts	SSHV Optical Micros. (A)	Coarse Dichot Optical Micros. (B)	Fine Dichot by Diff. (A-B)	SSHV CMB	Fine Dichot CMB	Coarse Dichot CMB
Oil & Gas Combustion	Fuel Comb., Carbon	----	5.8	-.-	1.0	1.0	-.-	-.-	-.-
Wood Combustion	----	Wood Boiler	1.4	-.-	-.-	-.-	-.-	8.6	3.0
Coal Combustion	Fuel Comb.,Part.Pyr.Coal	Coal-fired Power Plant	0.8	8.6	3.8	4.8	2.0	-.-	6.6
----	St.Mill, Part. Pyr. Coal	----	-.-	5.8	0.4	5.4	-.-	-.-	-.-
Coke	Steel Mill, Coke	Coke Ash	0.4	7.0	4.4	2.6	12.4	39.6	-.-
Steel	Steel Mill	Blast Furnace	2.0	34.6	12.4	22.2	16.4	-.-	-.-
----	----	Basic Oxygen Furnace	-.-	-.-	-.-	-.-	5.6	13.2	8.4
Coal	Coal Handling	----	0.8	4.6	2.8	1.8	-.-	-.-	-.-
Agricultural Products	Agr. Prod. Handling	----	5.4	6.0	-.-	6.0	-.-	-.-	-.-
Paint Products	Spray Painting	----	1.2	-.-	-.-	-.-	-.-	-.-	-.-
Cement, Limestone	Cement Handling	----	2.0	-.-	-.-	-.-	-.-	-.-	-.-
Lead	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Sand, Bentonite	Clay Handling	----	-.-	-.-	1.4	1.4	-.-	-.-	-.-
Aluminum	Alumina Handling	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Zinc	----	----	2.6	-.-	-.-	-.-	-.-	-.-	-.-
Misc. Chemicals	----	----	4.4	-.-	-.-	-.-	-.-	-.-	-.-
Refinery Catalysts	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Misc. Refinery	Oil Refining	----	3.2	-.-	-.-	-.-	-.-	-.-	-.-
Fertilizer	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Tire Products	----	----	8.6	-.-	-.-	-.-	-.-	-.-	-.-
----	Traffic, Tire Fragments	----	-.-	3.2	2.2	1.0	-.-	-.-	-.-
----	Traffic, Olum Carbon	Automobile Exhaust	-.-	5.0	2.8	2.2	4.4	1.0	0.8
Road Dust	Traffic, Wind Erosion	Near Street 1	32.2	41.2	17.4	23.8	25.2	2.0	75.2
----	Biologicals & Misc.	----	-.-	-.-	5.2	5.2	-.-	-.-	-.-
----	Secondary Aerosols	Secondary $(NH_4)_2SO_4$	-.-	27.6	5.3	22.3	27.5	24.4	3.0
Background	----	----	31.0	-.-	-.-	-.-	-.-	-.-	-.-
Total	----	----	101.8	143.6	59.1	99.7	93.5	88.8	97.1
Measured $PM_{2.5}$	----	----	99.8	-.-	-.-	99.8	-.-	99.8	-.-
Measured $PM_{2.5-10}$	----	----	65.4	-.-	65.4	-.-	-.-	-.-	65.4
Measured Dichot. PM_{10}	----	----	165.2	-.-	-.-	-.-	-.-	-.-	-.-
Measured SSHV PM_{10}	----	----	163.2	163.2	-.-	-.-	163.2	-.-	-.-

TABLE A-4

COMPARISON OF THE RECEPTOR AND DISPERSION MODEL RESULTS FOR THE OCTOBER 25, 1983 PM_{10} SAMPLES

Dispersion Modeling Source Groups	Optical Microscopy Source Categories	CMB Modeling Source Types	Modeled Concentrations ($\mu g/m^3$)						
			Dispersion Modeled Impacts	Optical Microscopy					
				SSHV	Fine Dichot	Coarse Dichot	SSHV CMB	Fine Dichot CMB	Coarse Dichot CMB
Oil & Gas Combustion	Fuel Comb., Carbon	----	0.4	-.-	1.0	0.4	-.-	-.-	-.-
Wood Combustion	----	Wood Boiler	-.-	-.-	-.-	-.-	-.-	6.8	0.6
Coal Combustion	Fuel Comb.,Part.Pyr.Coal	Coal-fired Power Plant	-.-	1.8	1.8	1.2	-.-	-.-	-.-
----	St.Mill, Part. Pyr. Coal	----	-.-	2.4	0.6	0.1	-.-	-.-	-.-
Coke	Steel Mill, Coke	Coke Ash	-.-	3.0	2.8	1.6	11.8	-.-	-.-
Steel	Steel Mill	Blast Furnace	-.-	5.4	5.8	1.0	10.6	-.-	5.0
----	----	Basic Oxygen Furnace	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Coal	Coal Handling	----	-.-	3.0	2.2	1.0	-.-	-.-	-.-
Agricultural Product	Agr. Prod. Handling	----	1.0	3.4	2.6	2.6	-.-	-.-	-.-
Paint Products	Spray Painting	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Cement, Limestone	Cement Handling	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Lead	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Sand, Bentonite	Clay Handling	----	0.6	-.-	-.-	-.-	-.-	-.-	-.-
Aluminum	Alumina Processing	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Zinc	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Misc. Chemicals	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Refinery Catalysts	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Misc. Refinery	Oil Refining	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Fertilizer	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
Tire Products	----	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
----	Traffic, Tire Fragments	----	-.-	1.2	1.0	0.6	-.-	-.-	-.-
----	Traffic, Clum Carbon	Automobile Exhaust	-.-	2.4	1.2	1.6	2.8	4.6	2.0
Road Dust	Traffic, Wind Erosion	Near Street 1	41.2	40.2	10.2	5.4	7.4	-.-	20.6
----	Biologicals & Misc.	----	-.-	-.-	-.-	-.-	-.-	-.-	-.-
----	Secondary Aerosols	Secondary $(NH_4)_2SO_4$	-.-	8.0	1.0	4.4	5.4	4.4	0.8
Background	----	----	17.0	-.-	-.-	-.-	-.-	-.-	-.-
Total	----	----	60.2	70.8	30.2	19.9	38.1	15.8	29.6
Measured $PM_{2.5}$	----	----	19.9	-.-	-.-	19.9	-.-	19.9	-.-
Measured $PM_{2.5-10}$	----	----	30.2	-.-	30.2	-.-	-.-	-.-	30.2
Measured Dichot. PM_{10}	----	----	50.1	-.-	-.-	-.-	-.-	-.-	-.-
Measured SSHV PM_{10}	----	----	70.8	70.8	-.-	-.-	70.8	-.-	-.-

between the time it was weighed and the time it was analyzed. Further evaluation of the sample indicated that this was indeed true. Thus, the correct mass was used to recompute the road dust profile.

The CMB model was rerun with the revised road dust profile and good agreement was now found between CMB and ISCST with respect to the combined impacts of road dust and vehicle exhaust. The CMB estimated impacts of the other sources remained unchanged by the revised road dust profile. Finally, the other source samples were re-weighed and no other cases of significant mass loss were identified.

Step 5 - Recompare Results After Rerunning CMB

The CMB model was rerun, the results were recompared and no significant difference in model estimates remained.

Step 6 - Refine Dispersion Model Inputs and Rerun

Case 2. A significant disagreement exists between the CMB and ISCST estimates of the coal combustion impacts.

The first step taken in reconciling the coal combustion impact estimates was to review the ambient and source composition data for errors which could potentially invalidate the CMB results. This review uncovered no obvious errors in the CMB input data related to coal combustion. The next step was to re-examine the comparisons between OM, CMB, and ISCST which are shown in Tables A-3 and A-4. These tables show that OM predicts coal combustion impacts in reasonable agreement with CMB and larger than ISCST. The emission inventory was then reviewed with respect to coal combustion sources. The review identified four major coal combustion facilities. For the closest of

these sources to the receptor, the emission inventory contained a very high value for the efficiency of the emission controls. Discussions with the plant personnel revealed that the inventory contained an erroneous value and a correct value was obtained. ISCST was then rerun with the corrected inventory and much closer agreement was found between CMB and ISCST with respect to coal combustion impacts.

Case 3. CMB estimates wood-fired boilers are a much larger contributor to PM_{10} than does ISCST.

The first step in reconciling the CMB and ISCST estimates for the wood-fired boiler impacts was to review the CMB input data. The review did not identify any obvious errors in the data. Next, the OM results were examined. In this case, OM was of little assistance because OM did not identify any impact from wood-fired boilers while CMB and ISCST both did. The emission inventory was then evaluated in terms of wood-fired boilers. There were no obvious problems found for the two wood-fired boiler sources in the inventory. Therefore, a site visit was conducted to each of the two plants. The site visits identified the possibility that one of the wood-fired boilers, located at a lumber mill, could be emitting particulate matter at a much higher rate than was listed in the inventory. Therefore, emission testing was conducted at the mill. The emission testing demonstrated that the emission inventory had severely underestimated the emission rate of the wood-fired boiler located at the lumber mill. ISCST was then rerun with the revised emission rate for the lumber mill boiler and good agreement was found between CMB and ISCST with respect to the wood-fired boiler source category.

Case 4. There is a big disagreement between CMB and ISCST for steel mill related impacts (i.e., coking operations, blast furnace, and basic oxygen furnace source categories).

The steel mill source is of additional interest due to the fact that there is a big disagreement between CMB and ISCST for each of the three main PM_{10} emitting activities within the steel mill. This disagreement results in CMB predicting that the steel mill is the largest industrial source of the PM_{10} levels observed at the receptor site while ISCST predicts that the steel mill is a relatively minor source. This discrepancy will have a big impact on control strategy development and therefore must be reconciled very carefully.

The first step in the reconciliation process was to review the CMB input data. The review did not identify any obvious anomalies in the CMB input data. In fact, the steel mill related source profiles were judged to be of very good quality due to the close agreement which was found between the plasma emission spectroscopy analysis of the resuspended samples which were collected on quartz fiber and the XRF analysis of those collected on Teflon. The next step was to examine the OM estimated impacts for the steel mill. In this case, OM was found to agree much better with CMB than with ISCST. The emission inventory was then reviewed with respect to steel mill emissions. The stack emission rates were found to be in good agreement with emission rates for similar activities at other steel mills. However, the review revealed that the emission inventory did not contain any fugitive emissions from the steel plant. This omission was viewed as a potentially serious deficiency; and, therefore, a site visit was conducted to reassess the stack and fugitive emission rates at the steel mill. The results of the stack testing were in good agreement with the original stack related emission

rates. However, substantial fugitive emissions were found to be associated with the coking operations, blast furnace, and basic oxygen furnace. ISCST was then rerun with the new fugitive emissions for the steel plant included in the inventory. This resulted in very good agreement between CMB and ISCST with respect to the steel mill contribution.

Step 7 - Recompare Results and Evaluate the Dispersion Model

The previous section presented the reconciliation of the CMB and ISCST source impact estimates and resulted in a number of revisions to the input data used by the models. Following Step 4, the CMB was rerun and after Step 6, the ISCST was rerun for subsets A and B using the revised data. The results obtained using the revised data are shown in Table A-5. Good agreement now exists between the source impacts estimated by CMB and ISCST for subsets A and B. Comparison of the ISCST results for subset A with the observed minus background concentrations is also significantly improved. ISCST was then run using 5 years of meteorological data to obtain estimates of the annual average PM_{10} and the six highest values. The results provided by ISCST are shown in Table A-6. ISCST predicts that both the annual average and 24-hour PM_{10} NAAQS will be exceeded at the monitoring station. Steel mill related activities are the major contributors to PM_{10} at the receptor site. The second largest contributor is resuspended road dust. The highest predicted PM_{10} concentrations all occur with persistent south winds, which further substantiates the steel mill contributions.

Step 8 - Final Model Estimates

The dispersion model results have been improved after extensive interaction with the CMB results. Thus, the dispersion model results in Table A-6 would be used for control strategy development.

TABLE A-5

COMPARISON OF FINAL VALIDATION RESULTS BY ISCST AND CMB FOR SUBSETS A AND B (ug/m^3)

Source Categories	(Representing Annual) Subset A ISCST	CMB	(Avg. of 5 24-hr runs) Subset B ISCST	CMB
Oil & Gas Combustion	1.6	--	2.0	--
Wood-fired Boilers	3.5	3.4 (1.6)	6.8	5.5 (2.2)
Coal Combustion	2.3	2.6 (1.4)	9.2	8.2 (3.0)
Coking Operations	10.1	8.4 (3.7)	19.0	22.0 (8.5)
Blast Furnace[a]	14.9	11.6 (2.5)	41.0	31.6 (6.9)
Basic Oxygen Furnace[a]		3.8 (1.7)		10.4 (2.6)
Coal Handling	0.3	--	0.6	--
Agricultural Prod. Handling	1.1	--	1.6	--
Paint Production	--	--	0.8	--
Cement & Limestone	1.9	--	1.9	--
Sand & Bentonite	1.2	--	1.7	--
Aluminum Production	--	--	0.4	--
Zinc Processing	0.8	--	0.6	--
Oil Refining	0.6	--	1.6	--
Fertilizer	--	--	0.8	--
Tire Production	--	--	2.2	--
Motor Vehicle Exhaust	15.1	2.2 (0.6)	2.6	2.6 (0.8)
Road Dust & Soil		15.1 (3.4)	31.2	39.2 (8.1)
Secondary $(NH_4)_2SO_4$	--	15.5 (2.7)	--	28.6 (4.4)
Background	15.0		32.0	--
Total	68.4	62.6	157.0	148.1
Measured	67.0	67.0	162.0	162.0

[a] estimated as a composite by the ISCST

NOTE: Numbers in parentheses indicate one standard error in the CBM analysis.

TABLE A-6

SOURCE CONTRIBUTIONS ESTIMATED BY ISCST USING 5 YEARS OF METEOROLOGICAL DATA (ug/m^3)

Source Categories	Annual Average	24-hr 6th Hiynest Concentration
Oil & Gas Combustion	1.4	1.7
Wood-fired Boilers	3.0	6.0
Coal Combustion	2.0	7.5
Coking Operations	8.7	27.6
Blast Furnace	10.1	38.0
Basic Oxygen Furnace	2.7	14.8
Coal Handling	0.3	0.4
Agricultural Prod. Handling	0.9	0.4
Paint Production	0.1	1.1
Cement & Limestone	1.6	2.1
Sand & Bentonite	1.0	0.7
Aluminum Production	0.1	0.2
Zinc Processing	0.6	0.6
Oil Refining	0.3	2.1
Fertilizer	0.1	0.9
Tire Production	0.4	1.5
Motor Vehicle Exhaust	12.7	45.4
Road Dust & Soil Background	15.0	32.0
Total	61.0	183.0